CAPEC Property Estimation Package

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The CAPEC Property Estimation Package has been designed and implemented to serve various activities in Computer Aided Process Engineering problems. At each step of process engineering problems, the package can be used as an analysis tool or simply providing property values during calculations.

The following software components are currently available in the CAPEC Property Estimation Package:

1. Pure Component Estimation Program (ProPred 3.5) including among others the following features:
    - Multilevel group-contribution method for the estimation of an important number of properties (melting point, normal boiling point, critical constants, octanol/water, partition coefficient, water solubility, toxicity, etc.) for a wide range of chemical compounds.
    - Prediction of functional properties (vapor pressure, density, viscosity and others) for a wide range of temperatures.
    - Regression module for fitting functional properties to several correlation equation models.

2. Thermodynamic Model Library (TML) including among others the following features:
    - Implementation of most-widely used thermodynamic models of excess Gibbs free energy and EOS.
    - Thermodynamic model selection guide.
    - Regression of model parameters (GE models, EOS models, mixture and pure component correlations).
    - Utility calculations, phase diagrams and model validation features.

3. Property Database includes:
    - Pure component and mixture properties.
    - Communication with other software components in CAPEC package.